Attorney Docket No.: 020910-000110US

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of:	Examiner: Unassigned
Michael A. Sherman, et al.	Art Unit: 1644
Application No.: 10/053,253	SUPPLEMENTAL INFORMATION
Filed: November 2, 2001	DISCLOSURE STATEMENT UNDER 37 CFR §1.97 and §1.98
For: METHOD FOR LARGE TIMESTEPS IN MOLECULAR MODELING	

Assistant Commissioner for Patents
Washington, D.C. 20231

Sir:

The references cited on attached form PTO/SB/08A and PTO/SB/08B are being called to the attention of the Examiner. Copies of the references are enclosed. It is respectfully requested that the cited references be expressly considered during the prosecution of this application, and the references be made of record therein and appear among the "references cited" on any patent to issue therefrom.

As provided for by 37 CFR 1.97(g) and (h), no representation is being made that a search has been conducted or that this statement encompasses all the possible relevant information, and no inference should be made that the information and references cited are, or are considered to be material to patentability because they are in this statement. No inference should be made that the information and references cited are prior art merely because they are in this statement.

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PATENT

   Applicant believes that <u>no fee is required</u> for submission of this statement.

However, if a fee is required, the Commissioner is authorized to deduct such fee from the

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        Respectfully submitted,

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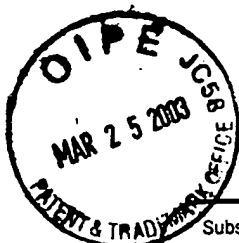
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Substitute for form 1449A/PTO			C mplete if Kn wn	
INFORMATION DISCLOSURE STATEMENT BY APPLICANT *(use as many sheets as necessary)*			Application Number	10/053,253
			Filing Date	November 2, 2001
			First Named Inventor	Sherman, Michael A.
			Art Unit	1644
			Examiner Name	Unassigned
Sheet	1	of 4	Attorney Docket Number	020910-000110US

U.S. PATENT DOCUMENTS

Examiner	Cite No.[1]	Document Number — Number Kind Code[2] (if known)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear
	AA	US 6,512,997	1/28/2003	Padilla, et al.	
	AB	US 6,253,166	6/26/2001	Whitmore, et al.	
	AC	US 6,185,506	2/6/2001	Cramer, III, et al.	
	AD	US 6,161,080	12/12/2000	Aouni-Ateshian, et al.	
	AE	US 6,150,179	11/21/2000	Went	
	AF	US 6,125,235	9/26/2000	Padilla, et al.	
	AG	US 6,081,766	6/27/2000	Chapman, et al.	
	AH	US 6,014,449	1/11/2000	Jacobs, et al.	
	AI	US 5,799,312	8/25/1998	Rigoutsos	
	AJ	US 5,787,279	7/28/1998	Rigoutsos	
	AK	US 5,777,889	7/7/1998	Mohanty, et al..	
	AL	US 5,752,019	5/12/1998	Rigoutsos, et al.	
	AM	US 5,745,385	4/28/1998	Hinsberg, III, et al.	
	AN	US 5,625,575	4/29/1997	Goyal, et al.	
	AO	US 5,553,004	9/3/1996	Gronbech-Jensen, et al.	
	AP	US 5,307,287	4/26/1994	Cramer, III, et al.	

FOREIGN PATENT DOCUMENTS

Examiner Initials*	Cite No.[1]	Foreign Patent Document — Country Code[3]	Number[4]	Kind Code[5] (if known)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear	T[6]
	AQ	WO	02/073334	A2	07-26-1990	Padilla, et al.		☐
	AR	WO	01/67310	A1	12-12-1991	Smith, et al.		☐
	AS	WO	96/24902	A1	04-01-1993	Wertz		☐

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*EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.

[1] Applicant's unique citation designation number (optional). [2] Kind Codes of U.S. Patent Documents at www.uspto.gov or MPEP 901.04. [3] Enter Office that issued the document, by the two-letter code (WIPO Standard ST.3). [4] For Japanese patent documents, the indication of the year of the reign of the Emperor must precede the serial number of the patent document. [5] Kind of document by the appropriate symbols as indicated on the document under WIPO Standard ST. 16 if possible. [6] Applicant is to place a check mark here if English language Translation is attached.

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			Art Unit	1644	
			Examiner Name	Unassigned	
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OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS

Examiner Initials *	Cite No.[1]	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T[2]
	AT	ASCHER, et al., Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations, 1998, pgs. 3-122 and 231-297, SIAM, Philadelphia, PA.	
	AU	BARAFF, et al., "*Large steps in cloth simulation*", 1998, Computer Graphics Proceedings SIGGRAPH 98 (Orlando, July 19-24) p43.pdf	
	AV	BARTH, et al., "*A separating framework for increasing the timestep in molecular dynamics*" in Computer Simulation of Biomolecular Systems - Theoretical and Experimental Applications, Volume 3, 1997, pgs. 97-121, Kluwer AcademicDordrecht, The Netherlands.	
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	AX	BISCHOF, et al., ADIFOR 2.0 Users' Guide, 1998, Argonne National Laboratory, University of Chicago, Argonne, IL.	
	AY	BRENAN, et al., Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations, 1989, Chapter 5 (pgs. 115-148), Elsevier Science Publishing Co., New York, NY.	
	AZ	BUTCHER, "*Towards efficient implementation of singly-implicit methods*", 1988, AMC Transactions of Mathematical Software 14:68-75.	
	BA	BYSTROFF, "*An alternative derivation of the equations of motion in torsion space for a branched linear chain*", 2001, Protein Engineering 14:825-828.	
	BB	COLEMAN, et al., "*The efficient computation of sparse Jacobian matrices using automatic differentiation*", 1996, Cornell Theory Center Technical Report CTC95TR225.	
	BC	EICHBERGER, et al., "*The benefits of parallel multibody simulation*", 1994, International Journal for Numerical Methods in Engineering, 37:1557-1572.	
	BD	GOLUB, et al., "*The Differentiation of Pseudo-Inverses and Non-Linear Least Squares Problems Whose Variables Separate*", 1973, SIAM J. Numer Anal. 10:413.	
	BE	HAIRER, et al., Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems, 2nd ed., 1996, Springer-Verlang, Germany.	
	BF	HE, et al., "*Macromolecular conformational dynamics in torsional angle space*", 1998, Journal of Chemical Physics 108:271.	
	BG	HOLLARS, et al., SD/FAST User's Manual, Version B.2, 1994, Symbolic Dynamics, California.	

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Sheet	3	of	4	Attorney Docket Number	020910-000110US

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	BH	IZAGUIRRE, et al., "Longer Time Steps for Molecular Dynamics", 1999, J.Chem.Phys. 110:9853.	
	BI	KANE, Dynamics, 3rd ed., 1978, Stanford University, Stanford, California.	
	BJ	LEACH, Molecular Modelling Principles and Applications, 2nd ed., 1996, Chapter 6 (pgs. 303-352) Pearson Education Limited, England.	
	BK	MARTINS, et al., "*An automated method for sensitivity analysis using complex variables*", 2000, American Institute of Arenautics and Astronoautics, 2000-0689 p1	
	BL	MOROKUMA, et al., "*Model studies of the structures, reactivities, and reaction mechanisms of metalloenzymes*", 2001, IBM J. Res. & Dev. 45(3/4):367-395.	
	BM	NORSETT, et al., "*Embedded SDIRK-methods of basic order three*", 1984, BIT 24:634-646.	
	BN	PONDER, TINKER User's Guide, Version 3.8, October 2000, Washington University, St. Louis, MO.	
	BO	RAPAPORT, The Art of Molecular Dynamics Simulation, 1995, reprinted with corrections 1998, Chapter 3 (pgs. 42-77), Cambridge University Press, United Kingdom.	
	BP	SCHLICK, "*Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation*", 1997, Annu. Rev. Biophys. Biomol. Struct., 26:181-222.	
	BQ	SCHLICK, "*Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations*" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 227-262, Springer-Verlang, Germany.	
	BR	SCHLICK, Molecular Modeling and Simulation - An Interdisciplinary Guide, 2002, Chapter 13 and References, pgs. 419-462 and 561-619, Springer-Verlang, Germany.	
	BS	SHAMPINE, "*Implementation of implicit formulas for the solution of ODEs*", 1980, SIAM J. Sci. Stat. Comput. 1:103-118.	
	BT	VERLET, "*Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules*", 1967, Physical Review, 159(1):98-103.	
	BU	VON SCHWERIN, Multibody System Simulation, 1999, Springer-Verlang, Germany.	

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| Sheet | 4 | of | 4 |

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	BV	WU, et al., *"Constraint dynamics algorithm for simulation of semiflexible macromolecules"*, 1998, Journal of Computational Chemistry 19:1555-1566	
	BW	YEN, et al., *"On the numerical solution of constrained multibody dynamic systems"*, 1994, University of Minnesota AHPCRC 94-038.	

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